Fate Report for Case # P-19-0138

Fate Summary Statement

Fate Summary Statement: P-19-0138
FATE Estimations for hydrolysis product acid, MW [redacted]
S = Reacts
Hydrolysis Half life min
VP = 636 torr at 25 °C (NOMO5)
BP 30 °C (M)
POTW removal (%) = PMN 90-99 via hydrolysis; then Hyd Pdt [redacted] 0;
Hyd Pdt HF 60 via sorption
Time for complete ultimate aerobic biodeg Hyd Pdt [redacted] mo;
Hyd Pdt HF > mo
Sorption to soils/sediments Hyd Pdt [redacted] low; Hyd Pdt [redacted] moderate
PBT Potential PMN P1B1; Hyd Pdt [redacted] P3BU; Hyd Pdt [redacted] P3B1
FATE Migration to ground water PMN negl; Hyd Pdt [redacted] rapid;
Hyd Pdt [redacted] moderate

Analogue found (include identifier and database)

Relevant Structure(s)
Water [redacted] product and HF
Landfill [redacted] product and HF
Air / Incineration Parent
Parent % incineration 99 9% (hazardous waste incinerator)

Environmental Fate Determination

PMN # P 19 0138
Summary: EPA estimated that the new chemical substance could have limited persistence and a low potential for bioaccumulation, such that repeated exposures are not expected to cause food-chain effects via accumulation in exposed organisms The hydrolysis product ([redacted] is estimated to be very persistent in the environment and its bioaccumulation potential is unknown; therefore, it is not known whether repeated exposures to it will cause food chain effects via accumulation in exposed organisms. Although EPA estimated that the hydrolysis product ([redacted]

could be very persistent, the substance has a low potential for bioaccumulation, such that repeated exposures are not expected to cause food-chain effects via accumulation in exposed organisms.

Fate: Environmental fate is the determination of which environmental compartment(s) a chemical moves to, the expected residence time in the environmental compartment(s) and removal and degradation processes. Environmental fate is an important factor in determining exposure and thus in determining whether a chemical may present an unreasonable risk. EPA estimated physical/chemical and fate properties of the new chemical substance using data for analogues (of the hydrolysis product (using data for analogue(s) (and data submitted for the hydrolysis product; and of the hydrolysis product (using data available for and fluoride ions. In wastewater treatment, the new chemical substance is expected to be removed with an efficiency of 90% to 99% due to rapid hydrolysis, the hydrolysis product (is expected to be removed with an efficiency of 0% due to low biodegradability, low sorption, and low stripping, and the hydrolysis product (is expected to be removed with an efficiency of 60% due to sorption. Removal of the hydrolysis products (and by biodegradation is negligible. Sorption of the hydrolysis product (to sludge, soil, and sediment is expected to be low and sorption of the hydrolysis product (to sludge, soil, and sediment is expected to be moderate. Migration of the new chemical substance to groundwater is expected to be negligible due to rapid hydrolysis, migration of the hydrolysis product (to groundwater is expected to be rapid due to low sorption to soil and sediment, and migration of the hydrolysis product (to groundwater is expected to be moderate due to moderate sorption to soil and sediment. Due to low estimated vapor pressure and Henry's law constant, the new chemical substance and the hydrolysis product (are expected to undergo negligible volatilization to air. Due to low reported vapor pressure, the hydrolysis product (is expected to undergo negligible volatilization to air. Overall, these estimates indicate that the new chemical substance has low potential to volatilize to air or migrate to groundwater; that the hydrolysis product (has low potential to volatilize to air and has high potential to migrate to groundwater; and that the hydrolysis product (has low potential to volatilize to air and has moderate potential to migrate to groundwater.

Persistence : Persistence is relevant to whether a new chemical substance is likely to present an unreasonable risk because chemicals that are not degraded in the environment at rates that prevent substantial buildup in the environment, and thus increase potential for exposure, may present a risk if the substance presents a hazard to human health or the environment. EPA estimated degradation half-lives of the new chemical substance using data

for analogues ([redacted] of the hydrolysis product ([redacted] using data for analogue(s) ([redacted] and of the hydrolysis product ([redacted] using data available for [redacted] EPA estimated that the new chemical substance's hydrolysis half-life is seconds; that the hydrolysis products' ([redacted] and [redacted] aerobic and anaerobic biodegradation half-lives are > 6 months. These estimates indicate that the new chemical substance may have limited persistence in aerobic environments (e.g., surface water) and anaerobic environments (e.g., sediments) due to hydrolysis. Further, these estimates indicate that the hydrolysis products ([redacted] and [redacted] may be very persistent in aerobic environments (e.g., surface water) and anaerobic environments (e.g., sediment).

Bioaccumulation : Bioaccumulation is relevant to whether a new chemical substance is likely to present an unreasonable risk because substances that bioaccumulate in aquatic and/or terrestrial species pose the potential for elevated exposures to humans and other organisms via food chains. EPA estimated the potential for the new chemical substance to bioaccumulate using data for analogues ([redacted] and of the hydrolysis product ([redacted] to bioaccumulate using data for fluoride ions. EPA estimated that the new chemical substance has low bioaccumulation potential based on rapid hydrolysis, the hydrolysis product ([redacted] has unknown bioaccumulation potential based on bioconcentration or bioaccumulation data reported for [redacted] and the hydrolysis product ([redacted] has low bioaccumulation potential based on fluoride, which is a nutrient. EPA estimated that the new chemical substance could have limited persistence and a low potential for bioaccumulation, such that repeated exposures are not expected to cause food-chain effects via accumulation in exposed organisms. The hydrolysis product ([redacted] is estimated to be very persistent in the environment and its bioaccumulation potential is unknown; therefore, it is not known whether repeated exposures to it will cause food chain effects via accumulation in exposed organisms. Although EPA estimated that the hydrolysis product ([redacted] could be very persistent, the substance has a low potential for bioaccumulation, such that repeated exposures are not expected to cause food-chain effects via accumulation in exposed organisms.

CBI: [redacted]
Fate Assessor: Card, Marcella
SMILES: [redacted]

Physical Properties

Property	Measured/Calculated Value	EPI
Molecular Form:	[redacted]	[redacted]
Molecular Wt.:		[redacted] g/mol
% < 500:		
% < 1000:		

Property	Measured Value	Method	Estimated Value	Method	EPI
Melting Point:					
Boiling Point:	[redacted]				
BP Pressure:					
Vapor Pressure:			[redacted]		
Water Solubility:					
Log P:					
Log Kow:					
Log Koc:	NaN				
Log BCF:					
Henry's Law:					

pH:	
pH Comment:	

Fate Analysis

Hydrolysis (t1/2, da):	Volatilization (t1/2) - River (hr):	Volatilization (t1/2) - Lake (da):
Atm Ox Potential (t1/2)OH (hr):	Atm Ox Potential (t1/2)O3 (hr):	Atm Ox Potential(t1/2) Total (hr):
MITI Linear:	MITI NonLinear:	
Biodeg Linear:	Biodeg NonLinear:	
Biodeg Survey ult:	Biodeg Survey Prim:	
STP (% removal) Total:	STP (% removal) Biodeg:	
STP (% removal)	STP (% removal)	

Ads:	Air:

Rationales

Removal in Wastewater Treatment:	
Atmospheric Oxidation:	
Hydrolysis:	
Photolysis:	
Aerobic Biodegradation:	
Anaerobic Biodegradation:	
Sorption to Soil and Sediment:	
Migration to Groundwater:	
Persistence - Air:	
Persistence - Water:	
Volatilization from Water:	
Soil:	
Sediment:	
Other:	
Standard:	
Bioaccumulation:	

PBT Ratings

Persistence	Bioaccumulation	Toxicity	PBT Comments
1	1	1	PMN
3	U	2 (ECO, HH)	Hyd Pdt [redacted]
3	1	2 (HH)	Hyd Pdt [redacted]

Exposure-Based Testing

Exposure-Based Testing:	

Fate Ratings

Removal in WWT/POTW (Overall):

Removal in WWT/POTW (Overall):	90-99;0;60 PMN;Hyd Pdt [redacted] Hyd Pdt [redacted]

Condition	Rating Values	Rating Description				Comment
		1	2	3	4	
WWT/POTW Sorption:	;1;2	Low	Moderate	Strong	V. Strong	PMN;Hyd Pdt [redacted] Hyd Pdt [redacted]
WWT/POTW Stripping:	4;4;4	Extensive	Moderate	Low	Negligible	PMN;Hyd Pdt [redacted] Hyd Pdt [redacted]
Biodegradation Removal:	;4;4	Unknown	High	Moderate	Negligible	
Biodegradation Destruction:		Unknown	Complete	Partial	—	
Aerobic Biodeg Ult:	;4;4	<= Days	Weeks	Months	> Months	PMN;Hyd Pdt [redacted] Hyd Pdt [redacted]
Aerobic Biodeg Prim:		<= Days	Weeks	Months	> Months	
Anaerobic Biodeg Ult:	;4;4	<= Days	Weeks	Months	> Months	PMN;Hyd Pdt [redacted] Hyd Pdt [redacted]
Anaerobic Biodeg Prim:		<= Days	Weeks	Months	> Months	

Condition	Rating Values	Rating Description				Comment
		1	2	3	4	
Hydrolysis (t1/2 at pH 7,25C) A:	1	<= Minutes	Hours	Days	>= Months	RC(=O)-F
Hydrolysis (t1/2 at pH 7,25C) B:		<= Minutes	Hours	Days	>= Months	
Sorption to Soils/Sediments:	;4;3	V. Strong	Strong	Moderate	Low	PMN;Hyd Pdt [redacted] Hyd Pdt [redacted]
Migration to Ground Water:	1;4;3	Negligible	Slow	Moderate	Rapid	PMN;Hyd Pdt [redacted] Hyd Pdt [redacted]
Photolysis A, Direct:		Negligible	Slow	Moderate	Rapid	
Photolysis B, Indirect:		Negligible	Slow	Moderate	Rapid	
Atmospheric Ox A, OH:		Negligible	Slow	Moderate	Rapid	
Atmospheric Ox B, O3:		Negligible	Slow	Moderate	Rapid	

Bio Comments:

Bio Comments: Fate Study Summaries are available.
The substance will hydrolyze (sec) to yield [redacted] and the [redacted]
The fugacity spreadsheet and the EPI output file for the carboxylic acid hydrolysis product of the PMN material are attached.

Fate Comments:

Fate Comments:

Comments/Telephone Log

Artifact	Update/Upload Time
[redacted]	[redacted]